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Final Report On: "Investigations on the usefulness of the Massively Parallel Processor for Study of Electronic Properties of Atomic and Condensed Matter Systems" (NAG 5836 from NASA Goddard Space Flight Center for the period 15 August 1986 to 14 August 1987.)

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This grant, which provided one half of the salary of a post-doctoral physicist was aimed at exploring the usefulness of the Massively Parallel Processor (MPP) at NASA Goddard Space Flight Center for investigation of electronic structures and hyperfine properties of atomic and condensed matter systems. Our major effort during this period was directed towards the preparation of algorithms for parallelization of the computational procedure we have been using on serial computers for electronic structure calculations in condensed matter systems. Before getting involved in the more complicated Hartree-Fock procedure, it was necessary for us, as outlined in the proposal, to gain experience in parallel computation using a simpler and approximate method termed Self-Consistent Charge Extended Huckel (SCCEH) method and to benchmark the performance of the MPP for our purposes as compared to the high-speed serial computer UNIVAC 1100/92 we have been using for our work over the past few years.

About four months of the grant period was spent in familiarizing ourselves with the language and operation of the MPP. The MPP was accessed from our University through the TELENET and SPAN networks. In the remainder of the period of the grant, one of our main accomplishments was the adaptation of a major component of the SCCEH method, namely, the evaluation of the matrix elements the Hamiltonian used in the variational procedure employed to determine the electronic wave-functions of large molecules and clusters of atoms. This experience helped us in developing a general algorithm for calculating two-center one electron integrals that occur in the Hartree-Fock procedure, which we are interested in carrying out on the MPP. Lastly, as described in the proposal, our many-body atomic investigations require fast evaluation of a very large number of two-electron integrals of the coulomb and exchange types involved in the matrix elements of the electron-electron interaction over ground and excited state wave-functions. These integrals are usually carried out by standard quadrature procedures for numerical integrations. Towards the end of the grant period, we explored the adaptation of Gaussian and Laguerre quadrature procedures to the MPP for calculations of such integrals.

Detailed descriptions of these investigations and results are described in the attached Appendix. These results were

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presented on 24 April 1987 before an internal panel of the Space Computing and Image Analysis Division of the NASA Goddard Space Flight Center consisting of Dr. Milt Halem, Mr. James Fischer and associates. An article based on these results will be prepared in the future after some additional investigations, which unfortunately have been slowed down by the non-availability of support for personnel to work on this project.

APPENDIX

The work reported in this Appendix represents the joint efforts of Dr. N. Sahoo (post-doctoral research associate), Department of Physics, SUNY Albany, Dr. S.N. Ray of Systems and Applied Science Corporation, Lanham, Maryland and Professor T.P. Das, Department of Physics, SUNY Albany.

A. MPP-ADAPTION OF SELF-CONSISTENT CHARGE EXTENDED HUCKEL (SCCEH) PROCEDURE

(I) The SCCEH Procedure

The Self-Consistent-Charge Extended Hückel (SCCEH) procedure^{1,2}, is a semi-empirical method to determine the electronic energy levels and wavefunctions of a molecule. This approach is based on the valence shell approximation where the one-electron Hamiltonian is defined only through its matrix elements in the atomic valence shell orbital basis. These matrix elements are not evaluated through explicit treatment of electron-electron interaction but by relating them to experimentally measured ionization energies of the pertinent atoms and ions.

In this method the molecular orbitals (MO) ψ_μ are expressed as a linear combination of atomic orbitals (AO) χ_i in the form

$$\psi_\mu = \sum_i c_{\mu i} \chi_i \quad (1)$$

in common with other LCAO procedures, the coefficients $c_{\mu i}$ representing MO coefficients which are treated as variational parameters for calculating the minimum energy configuration of the molecule. The values of $c_{\mu i}$ in the LCAOMO procedure for which the total energy is minimum are obtained by solving the secular equation:

$$\sum_j c_{\mu j} (H_{ij} - S_{ij} E_\mu) = 0 \quad (2)$$

where H_{ij} and S_{ij} in eq. (2) represent the Hamiltonian and overlap matrix elements respectively. The major computational steps involved in solving equation (2) for $c_{\mu i}$ (which in turn determines the ψ_μ from which all the electronic properties are calculated) and E_μ (the one electron energy levels) for the SCCEH procedure are the following.

1. Determination of H_{ij} :

The Hamiltonian matrix elements H_{ij} are constructed empirically from the orbital ionization energies ϵ_i determined from atomic data, and the charges q_ℓ on atom ℓ . The charge q_ℓ on any atom ℓ is obtained from the coefficients $c_{\mu i}$ by using the Mulliken approximation

$$q_\ell = -\sum_i (q_{\ell i}^\alpha + q_{\ell i}^\beta) + Z_\ell$$

with

$$q_{\ell i}^{\alpha, \beta} = \sum_\mu (|c_{\mu i}|^2 + \sum_{m \neq \ell} \sum_g^m c_{\mu i} c_{\mu g} S_{ig}) n_\mu^{\alpha, \beta} \quad (3)$$

where α and β represent spin states, $n_\mu^{\alpha, \beta}$ the populations of μ th occupied orbital for the two different spin states, and Z_ℓ represents the valence charge on atom ℓ .

The q_ℓ s are incorporated in H through the equations

$$H_{ii} = \epsilon_i^0 \pm |q_\ell| (\epsilon_i^\pm - \epsilon_i^0)$$

$$H_{ig} = \frac{k}{2} (H_{ii} + H_{gg}) S_{ig} \quad (4)$$

2. The determination of S_{ij} :

For the determination of H_{ij} one needs to evaluate S_{ij} , the overlap integral between atomic orbitals which is given by

$$S_{ij} = \int \chi_i^*(\vec{r}) \chi_j(\vec{r}) d\vec{r} \quad (5)$$

The atomic orbitals used in equations (1) and (5) are usually taken as Slater type orbitals³ (STO) but could equally well be taken as Gaussian type orbitals⁴ (GTO). The expression for an STO is given by

$$\chi_{iN}^{n\ell m}(r, \theta, \phi) = N_{iN} r_N^{n-1} e^{-\zeta_{iN} r_N} Y_{\ell m}(\theta, \phi) \quad (6)$$

and that for a GTO is given by

$$\chi_i^N(\vec{r}) = N_{iN} x_N^{a_i} y_N^{b_i} z_N^{c_i} e^{-\zeta_{iN} r_N^2} \quad (7)$$

with $a_1 + b_1 + c_1 = l_1$, the angular momentum of the atomic orbital. In equations (6) and (7), the exponents γ_{iN} are chosen from analysis of the nature and features of the wave-functions of the atoms involved in the molecular system studied.

The overlap integrals are the simplest two center integrals encountered in the molecular electronic structure calculations. Since the evaluation of these integrals between a pair of atomic orbitals are independent of each other, they can be computed in parallel.

(1) Overlap integrals over STOs-

The detailed formalism for numerical evaluation of overlap integrals for Slater type orbitals is documented in the literature⁵. After careful examination of different formulae involved in the evaluation of such integrals, we decided on a particular area where we can use the MPP very effectively. The expression for the two center overlap integral can be algebraically reduced to expressions involving one or more basic two center integrals, known as reduced overlap integrals. The reduced overlap integrals are finally expressed in terms of the auxiliary functions $A_k(\rho)$ and $B_k(\rho)$ which are evaluated using the following recurrence relations:

$$\rho A_k(\rho) = k A_{k-1}(\rho) + e^{-\rho} \quad (8)$$

where

$$\rho = \frac{\gamma_A R + \gamma_B R}{2} \quad (9)$$

and

$$B_k(x) = (-1)^{k+1} A_k(-x) - A_k(x) \quad (10)$$

and

$$x = \frac{\gamma_A R - \gamma_B R}{2} \quad (11)$$

The expression for $A_k(\rho)$ and $B_k(x)$ are given by

$$A_k(\rho) = \int_0^\infty x^k e^{-\rho x} dx, \quad (12)$$

$$B_k(x) = \int_{-1}^1 y^k e^{-xy} dy \quad (13)$$

In the above expressions R is the separation between atoms A and B , and ζ_A and ζ_B are the Slater exponents of any atomic orbital centered on atom A and B respectively.

The expressions (8-13) can be easily evaluated in the MPP with considerable saving of the computational time compared to a serial processor by using the following algorithm.

For 128 basis functions, involving different ζ_{IN} , irrespective of their angular momentum symmetry, ρ and X can be constructed as a 128×128 matrix. Thus $A_0(\rho)$ and $B_0(X)$ can be evaluated for 16,384 ρ or X values simultaneously or in parallel using the MPP. Once $A_0(\rho)$ and $B_0(X)$ are evaluated, the $A_k(\rho)$ and $B_k(X)$ for $k \neq 0$ can be obtained using the recursion relations (8) and (10). The $A_k(\rho)$ and $B_k(X)$ can be evaluated simultaneously for 16,384 values of ρ and X using the MPP. We have made substantial progress in programming this part in parallel pascal for MPP and the procedure will be called from the main FORTRAN program residing in host VAX memory. We have not done any benchmarking yet for these integrals, but we expect the computation in MPP will be much faster compared to the serial processor from our experience for overlap integrals using Gaussian orbitals described next. Our main motivation behind the analysis of overlap integrals involving Slater orbitals was to gain experience in redesigning parallel algorithms for recursive numerical procedures similar to the ones described above.

3. Overlap integrals over GTOs:

The MPP can be utilized more effectively for evaluation of molecular integrals in general and overlap integrals in particular when one uses Gaussian type of atomic basis functions. In this case, all the molecular integrals can be analytically expressed in terms of some basic integrals, which can be simultaneously evaluated using the MPP. We will describe first the evaluation of overlap integrals between Gaussian functions and in the following section discuss the generalization of this procedure for other one electron two center integrals.

The overlap integrals between two Gaussian type functions G_A and G_B , namely,

$$S_{AB} = \int_{-\infty}^{+\infty} G_A G_B dx dy dz \quad (14)$$

of any symmetry can be expressed⁶ in terms of overlap integral between two s-functions, $\langle S|S \rangle$ which is given by

$$\langle S|S \rangle = K N_A N_B (\pi/\gamma)^{3/2} \quad (15)$$

For example, the overlap integrals between p_z and s orbitals on two centers and between p_z and p_z orbitals on two adjacent centers A and B can be written in the form:

$$\langle z|s\rangle = -\frac{\gamma_B}{\gamma} (\overline{AB})_z \langle s|s\rangle \quad \text{and} \quad \langle z|z\rangle = \left(\frac{1}{2\gamma} - \frac{\gamma_A \gamma_B}{\gamma^2} (\overline{AB})_z^2\right) \langle s|s\rangle$$

In the above expressions,

$$K = e^{-(\gamma_A \gamma_B / (\gamma_A + \gamma_B)) (\overline{AB})^2} \quad (16)$$

where $(\overline{AB})^2$ is the square of the distance between two centers A and B, γ_A and γ_B are exponents in the Gaussian functions G_A and G_B , N_A and N_B are the normalization constants,

$$\gamma = \gamma_A + \gamma_B$$

and

$$(\overline{AB})_i = (\vec{A} - \vec{B})_i$$

The $\langle s|s\rangle$ integrals are evaluated in the MPP using the following steps.

- evaluate the distance matrix from which $(\overline{AB})^2$ is calculated.
- evaluate the $\gamma_A \gamma_B$ matrix
- evaluate the $\gamma_A + \gamma_B$ matrix
- evaluate the $N_A N_B$ matrix
- evaluate the K matrix

Since the MPP can do arithmetic operations involving 128×128 parallel arrays, the Gaussian functions are divided into blocks of 128 Gaussians and all the parallel arrays or matrices involved in the steps a-e have 128×128 array dimension.

As an example, we will describe the algorithm for the evaluation of the distance matrix for 128 points. For this purpose one first constructs three 128×128 parallel arrays with each column containing x , y or z coordinate of a single point. e.g.

$$[C]_{ni} = x_i, [D]_{ni} = y_i, [E]_{ni} = z_i \quad (17)$$

for $n=1, 128$ and $i=1, 128$.

For instance:

$$[C] = \begin{bmatrix} x_1 & x_2 & \dots & x_{128} \\ x_1 & x_2 & \dots & x_{128} \\ \vdots & \vdots & & \vdots \\ x_1 & x_2 & \dots & x_{128} \end{bmatrix} \quad (18)$$

with 128 rows.

One then calculates the transpose of matrices $[C]$, $[D]$, and $[E]$ from which

$$[x] = [c] - [c]^T, [y] = [D] - [D]^T, [z] = [E] - [E]^T \quad (19)$$

are obtained. One can easily see that

$$[x]_{ij} = x_i - x_j, [y]_{ij} = y_i - y_j \text{ and } [z]_{ij} = z_i - z_j \quad (20)$$

Therefore the distance matrix for different centers can be obtained from

$$[r]_{ij} = \sqrt{[x]_{ij} * [x]_{ij} + [y]_{ij} * [y]_{ij} + [z]_{ij} * [z]_{ij}} \quad (21)$$

In contrast to serial computation where the arithmetic operations are carried over one data item, like $x_i - x_j$, here we are evaluating the difference between x-coordinates of all the 128 centers simultaneously. This leads to considerable saving in computational time. A similar procedure is followed in carrying out the steps b to d. Once the matrices in (a), (b) and (c) have been evaluated, the matrix (e) can be obtained directly using Eq. (16). The parallel pascal programs for these steps have been written and tested on the MPP. It is straight forward to calculate the overlap integrals $\langle z|s \rangle$ and $\langle z|z \rangle$ from $\langle s|s \rangle$ using the equation (15). In actual molecular calculations, the atomic orbitals are expressed as linear combination of Gaussian functions like

$$\phi_i^A = \sum_p d_{pi}^A G_{pi}^A, \quad \phi_j^B = \sum_q d_{qj}^B G_{qj}^B \quad (22)$$

The overlap integral between ϕ_i^A and ϕ_j^B can then be written as

$$\langle \phi_i^A | \phi_j^B \rangle = \sum_p \sum_q d_p^A d_q^B \langle G_p^A | G_q^B \rangle \quad (23)$$

Equation (23) can also be evaluated on the MPP by computing $\langle G_p^A | G_q^B \rangle$, the overlap integrals between the primitives, and then multiplying it with the $d_p^A d_q^B$ matrices and performing the appropriate contracted sum.

Our bench-marking procedure has shown that these one electron two center integrals can be computed 15 times faster in MPP compared to UNIVAC 1100/91.

4. The Iterative Process:

After the evaluation of S_{ij} by a MPP resident routine, the H_{ii} and H_{jj} are evaluated from some initial charge state of the atoms and the secular equations (2) are solved to find out the for the next cycle. The solution of equations (2) requiring the diagonalization of a large matrix, which may be done faster on the MPP using suitable parallel algorithm than the existing serial codes. We have been working on developing a parallel

pascal code₇ for matrix diagonalization using available parallel algorithms.

The MO coefficients $C_{\mu i}$ thus obtained are used to determine from equation (3) and the new H_{ij} are constructed again using equations (4) and the whole process is repeated until the charge on each atom stabilizes within a chosen tolerance limit. $q_{ei}^{\alpha, \beta}$

A host resident routine is used to carry out the iterative process.

We have thus made considerable progress in adapting the existing serial code for SCCEH procedure into the MPP. The novel architecture of the MPP is exploited wherever it is possible at the present time.

(B) MPP ADAPTATION OF THE FIRST-PRINCIPLES HARTREE-FOCK CLUSTER PROCEDURE FOR ELECTRONIC STRUCTURES OF LARGE MOLECULES AND SOLID STATE SYSTEMS:

Our ultimate aim is to adapt to the MPP the first-principles linear-combinations of Atomic Orbitals-Molecular Orbital (LCAOMO) Hartree-Fock procedure to study the electronic structures of large molecules and atomic clusters used to stimulate solid state systems. Our experience in parallel evaluation of overlap integrals using the MPP has helped us to make some progress in this direction. The major computational effort involved in this procedure is the evaluation of $F_{\mu\nu}$, the matrix elements of the Hartree-Fock operator in the chosen atomic basis set which are given by⁹

$$\begin{aligned}
 F_{\mu\nu} = & \int \phi_{\mu}(1) \left(-\frac{\nabla_1^2}{2}\right) \phi_{\nu}(1) dx dy dz + \sum_{\text{J}} \int \phi_{\mu}(1) \left(-\frac{Z_{\text{J}}}{r_{1\text{J}}}\right) \phi_{\nu}(1) dx dy dz \\
 & + \sum_{\text{g}} \sum_{\lambda} \sum_{\sigma} C_{\text{g}\lambda} C_{\text{g}\sigma} \left[2 \int \phi_{\mu}(1) \phi_{\nu}(1) \frac{1}{r_{12}} \phi_{\lambda}(2) \phi_{\sigma}(2) dx_1 dy_1 dz_1 dx_2 dy_2 dz_2 \right. \\
 & \left. - \int \phi_{\mu}(1) \phi_{\lambda}(1) \frac{1}{r_{12}} \phi_{\nu}(2) \phi_{\sigma}(2) dx_1 dy_1 dz_1 dx_2 dy_2 dz_2 \right] \quad (24)
 \end{aligned}$$

In the above expression the first term is the kinetic energy integral, the second term is the potential energy integral and the third and fourth terms are the two electron coulomb and exchange integrals. The kinetic energy (K.E.)₆ integrals for Gaussian type atomic orbitals can be expressed in terms of the overlap integrals between S-type gaussian functions. The evaluation of such kinds of integrals by MPP has already been

described in Appendix A. We are now developing a parallel pascal code for the evaluation of these K.E. integrals from the overlap integrals. We plan to develop parallel pascal codes for other electronic integrals in the future.

The total energy of a cluster of atoms and ions used to simulate the infinite solid state system is the sum of electronic energy and the energy of repulsion (and attraction for opposite charges) V_{NN} between the charge on the ions. The electronic energy is obtained by solving a set of Hartree-Fock equations, whereas V_{NN} is calculated using the expression,

$$V_{NN} = \frac{1}{2} \sum_{i,j=1}^N \frac{Z_I Z_J}{|\vec{R}_I - \vec{R}_J|} \quad (25)$$

Z_I and R_I being respectively the charge and position vector of the I th ion.

We have written a parallel pascal code for the MPP following the algorithm described earlier for the evaluation of the distance matrix. We found that this can be done 30 times faster compared to the UNIVAC 1100/91 serial computer.

C. MPP Adaption of the Many-Body Procedure for Atomic Systems:

We have also been interested in adapting to the MPP the relativistic many-body procedure¹⁰ for studying properties of atomic systems. The most time-consuming computation in this procedure is that requiring the evaluation of the matrix elements of the electron-electron interaction involving three and four excited^{10,11} state wave functions of an atom of the form:

$$I_3 = \iint \psi_{k1}^*(1) \psi_{k2}^*(2) \frac{1}{r_{12}} \psi_{k3}(1) \psi_c(2) d^3r_1 d^3r_2$$

and

(26)

$$I_4 = \iint \psi_{k1}^*(1) \psi_{k2}^*(2) \frac{1}{r_{12}} \psi_{k3}(1) \psi_{k4}(2) d^3r_1 d^3r_2$$

In the above expression $k1, k2, k3$ and $k4$ refer to unoccupied one-electron excited states and c to one of the occupied one-electron states for the many-electron Dirac Hartree-Fock Hamiltonian.

Usually these integrals are evaluated following the standard numerical procedures like Laguerre integration¹² quadrature. To gain experience in designing parallel algorithms for numerical integrations, we have concentrated on writing MPP pascal codes for Laguerre quadrature involving simple functions. It will help us to develop suitable parallel codes for evaluation of I_3 and I_4 in equation (26). We will briefly describe the algorithm for the simultaneous evaluation of

$$I_j = \int_0^{\infty} g_j(x) dx \quad (27)$$

on the MPP, for 128 different functions g_j . The procedure can be easily generalized also for $j \neq 128$. If one uses the Laguerre integration formula¹², then equation (27) can be written as

$$I_j \approx \sum_{i=1}^n (w_i e^{x_i} g_j(x_i)) \approx \sum_{i=1}^n f_i^j(x_i) \quad (28)$$

where x_i are the zeros of Laguerre Polynomials, w_i are the weight factors. The number of terms n , in the summation is chosen depending on the desired accuracy. We will choose $n=128$ for the sake of clarity, but the procedure can be used for a smaller number of n values, as is normally done in this field. The x_i and $w_i e^{x_i}$ are available from standard tables¹² and can be stored on the MPP as data. Each column of the 128×128 array of the MPP will contain the 128 x_i and $w_i e^{x_i}$ values such that

$$[C]_{in} = x_i$$

and (29)

$$[D]_{in} = w_i e^{x_i}$$

for $n=1$ to 128 as in section 3 of Appendix A. In equations (29), $[C]$ and $[D]$ are 128×128 parallel array data items.

If all the $g_j(x)$ in Eqs. (27) and (28) have the same algebraic form differing only by values of some specific parameters, one can evaluate the values of $g_j(x_i)$ at 128 x_i values using the MPP. If they have different form, then one can use the host VAX computer to evaluate them and transfer them to the MPP. Let us assume that we have a parallel array data $[G]$, whose elements are

$$[G]_{kj} = g_j(x_k) \quad (30)$$

Now $[H]_{ij} = [C]_{ij} * [D]_{ij} * [G]_{ij}$ will give us the quantity $f_i(x_j)$ in Eq. (28) for all the 128 functions at the 128 x_i values.

Thus

$$[H]_{ij} = g_j(x_i) w_i e^{x_i} \quad \text{for 128 values of } i \text{ and } j.$$

From Eq. (28) it then follows that

$$I_j = \sum_i [H]_{ij} \quad (31)$$

This addition can be easily done by repeatedly using the predeclared shift functions in MPP pascal¹³ language and adding to the parallel array on which the shift operation is applied. Thus:

Suppose $[S]^1 = \text{shift}([S]^{1-1}, n_1, 0)$ where n_1 is chosen such that in each successive shift operations we north shift the parallel array by twice the number of rows of the previous shift operation, that is, $n_{i+1} = 2n_i$ until $n_{i+1} = 64$.

$$\text{Then, } [R] = \sum_{i=1}^7 [S]^{i-1} + [S]^i \quad (32)$$

where the resulting parallel array $[R]$ will be such that

$$[R]_{ij} = I_j \quad \text{for } j=1 \text{ to } 128 \text{ values.} \quad (33)$$

The number of arithmetic operations involved in carrying out the numerical integration of 128 functions by the above procedure is much less compared to the number of arithmetic operations involved in the serial computation. For example the evaluation of $[H]$ on MPP requires three multiplication operations compared to 49152 multiplications on serial computers. Similarly, in the summation in equation (28) for 128 functions, one needs only 7 addition operations compared to the 16384 required additions on serial computers. Thus numerical integration of large numbers of functions will be much faster on the MPP compared to the conventional serial processors. When one uses smaller numbers of zeros of Laguerre Polynomials in Eq. (28) one can increase the number j of functions to be integrated such that all the processors in the array are properly utilized. We hope to benchmark the performance of the MPP pascal program following the above procedure in the future.

D. CONCLUSION

In the past one year we have made progress in using the MPP efficiently for electronic structure calculations of atomic and solid state systems. It is a different computing environment than with the conventional serial computers used before and one has to redesign the parallel algorithms and rewrite computer codes to convert existing FORTRAN codes used for electronic structure calculations. Non-availability of a scientific subroutine library in MPP Pascal language makes the conversion more difficult and time consuming. Thus we will devote further efforts in the coming years to write suitable MPP Pascal

subprograms for many of the standard numerical procedures that are required for our investigations.

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